FEM Multigrid Techniques for Viscoelastic Flow

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Multiscale CFD Problems

Inertia turbulence

\[ \text{Re} \gg 1 \]

Numerical instabilities + problems

Turbulence Models

Stabilization Techniques

**Characteristics:**
- Irregular temporal behaviour and spatially disordered
- Broad range of spatial/temporal scales
Multiscale CFD Problems

Elastic turbulence

- $\text{Re} \ll 1, \text{Wi} > 1$ (less inertia, more elasticity)
- Coil stretching, high stresses
- Numerical instabilities + problems

Flow models: Oldroyd, Maxwell, ...
Stabilization: EEME, EEVS, DEVSS/DG, SD, SUPG, ...
Nonlinear Flow Models

Generalized Navier-Stokes equations

\[ \rho \frac{\partial u}{\partial t} + u \cdot \nabla u - \text{div} \, \sigma + \nabla p = \rho f, \quad \text{div} \, u = 0, \]

\[ \frac{\partial \Theta}{\partial t} + u \cdot \nabla \Theta - \text{div} \, k \nabla \Theta - D : \sigma = 0, \]

\[ \sigma = \sigma^s + \sigma^p, \quad D = \frac{1}{2} \left( \nabla u + \nabla u^T \right) \]

Quasi-Newtonian part \( \sigma^s = 2\eta_s (D, \Theta)D \)

Viscoelastic part \( \sigma^p + \Lambda \frac{\delta_a \sigma^p}{\delta t} = 2\eta_p D, \)

\[ \frac{\delta_a \sigma}{\delta t} = \left( \frac{\partial}{\partial t} + u \cdot \nabla \right) \sigma + \frac{1-a}{2} \left( \sigma \nabla u + \nabla u^T \sigma \right) \]

\[ - \frac{1+a}{2} \left( \nabla u \sigma + \sigma \nabla u^T \right) \]
Required: I) Special Models

\[ T + \Lambda \frac{\delta_a T}{\delta t} = 2\eta_0 \left( D + \Lambda_r \frac{\delta_a D}{\delta t} \right) \]

\[ T + \Lambda \frac{\delta_a T}{\delta t} + B(T) = 2\eta D \]

Oldroyd A
Oldroyd B
Maxwell A
Maxwell B
Jeffreys

Phan-Thien Tanner
Phan-Thien
Giesekus
Required: II) Special Numerics

- Special FEM Techniques
- Multigrid Solvers
- Stabilization for high Re and Wi Numbers
- Implicit Approaches
- Space-Time Adaptivity
- Grid Deformation Methods
- Newton Methods
Our Numerical Approach

Fully implicit monolithic multigrid FEM solver
Numerical Techniques

- The FEM techniques have to handle the following challenging points
  - Stable FE spaces for velocity and pressure fields, and velocity and extra-stress fields \( \rightarrow Q2/P1/? \) or \( Q1(nc)/P0/? \) (new: \( Q2(nc)/P1/? \))
  - Special treatment of the convective terms \( u \cdot \nabla u, \ u \cdot \nabla \Theta, \ u \cdot \nabla \sigma \)
    \( \rightarrow \) edge-oriented/interior penalty FEM, TVD/FCT
  - The presence of the "reactive" terms which are responsible for
    - high Weissenberg number problem (HWP) \( \rightarrow \) LCR
    - blow up phenomena for time dependent solution

- The (nonlinear) solvers have to deal with different source of nonlinearity
  - nonlinear viscosities \( \rightarrow \) Newton method via divided differences
  - the strong coupling of equations \( \rightarrow \) monolithic multigrid approach
  - complex geometries and meshes
Newton Solver

Solve for the residual of the nonlinear system algebraic equations

\[ R(x) = 0, \quad x = (u, \Theta, \sigma, p) \]

Newton method with damping results in iterations of the form

\[ x^{n+1} = x^n + \omega^n \left[ \frac{\partial R(x^n)}{\partial x} \right]^{-1} R(x^n) \]

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- Continuous Newton: on variational level (before discretization)
- The continuous Frechet operator can be calculated

- Inexact Newton: on matrix level (after discretization)
- The Jacobian matrix is \textbf{approximated} using finite differences as

\[
\begin{bmatrix}
\frac{\partial R(x^n)}{\partial x}
\end{bmatrix}_{ij} \approx \frac{R_i(x^n + \varepsilon_j) - R_i(x^n - \varepsilon_j)}{2\varepsilon}
\]
Multigrid Solver

- Standard geometric multigrid approach
- Full $Q_2$, $Q_1$, $P_1^{disc}$ and $P_0$ grid transfer
- Smoother: Local/Global MPSC
  - Local MPSC via Vanka-like smoother
    $$
    \begin{bmatrix}
    u^{l+1} \\
    \sigma^{l+1} \\
    \Theta^{l+1} \\
    p^{l+1}
    \end{bmatrix}
    =
    \begin{bmatrix}
    u^l \\
    \sigma^l \\
    \Theta^l \\
    p^l
    \end{bmatrix}
    + \omega^l \sum_{T \in T_h} [K + J]^{-1}_T \begin{bmatrix}
    \text{Res}_u \\
    \text{Res}_\sigma \\
    \text{Res}_\Theta \\
    \text{Res}_p
    \end{bmatrix}_T
    $$

  - Global MPSC
    - solve for an intermediate $\tilde{u}$ (generalized momentum equation)
    - solve for $p$ (pressure Poisson equation)
    - update of $u$ and $p$
    - solve for $\Theta$ (tracer equation)
    - solve for $\sigma$ (constitutive equation)

Coupled multigrid solver

Decoupled multigrid solver
Viscoelastic Models

Different highly developed models

Oldroyd A/B, Maxwell A/B, Jeffreys, PTT, Giesekus

...nevertheless, despite „good“ models and „good“ Numerics, the HWNP („High Weissenberg Number problem“) stills exists for critical Wi, resp., De numbers...

Kinetic Energy for two different velocity inflow

Zoom shows oscillation...!!
Problem Reformulation

Old $\rightarrow (u, p, \sigma^p)$
\[
\begin{align*}
\rho \left( \frac{\partial u}{\partial t} + u \cdot \nabla u \right) &= \nabla p - 2\eta_s \nabla \cdot D - \nabla \cdot \sigma^p, \\
\nabla \cdot u &= 0, \\
\Lambda \frac{\delta_a \sigma^p}{\delta t} + \sigma^p - 2\eta_p D &= 0,
\end{align*}
\]

(1)

Conformation tensor $\rightarrow (u, p, \tau)$

This tensor is positive definite by design !!

Replace $\sigma^p$ in (1) with $\sigma^p = \frac{\eta_p}{\Lambda} (\tau - I)$ $\rightarrow$ special discretization : TVD

\[
\begin{align*}
\rho \left( \frac{\partial u}{\partial t} + u \cdot \nabla u \right) &= \nabla p - 2\eta_s \nabla \cdot D - \frac{\eta_p}{\Lambda} \nabla \cdot \tau, \\
\nabla \cdot u &= 0, \\
\frac{\delta_a \tau}{\delta t} + \frac{1}{\Lambda} (\tau - I) &= 0,
\end{align*}
\]

(2)
Properties of Conformation Tensor

\[ \tau(X,t) = \int_{\infty}^{t} \eta_p \exp \left( \frac{-(t-s)}{\sqrt{\Lambda}} \right) F(s,t) F(s,t)^T ds \]

Positive by design, so we can take its logarithm

2 observations:
- positive definite \(\rightarrow\) special discretizations like FCT/TVD
- exponential behaviour \(\rightarrow\) approximation by polynomials???
Driven Cavity

Cutline of Stress_11 component at y = 1.0

Old Formulation Vs Lcr

Old: $\text{We}=0.5$ - $\text{We}=1.5$

(LCR)

(Old)
Problem Reformulation

M. Behr $\rightarrow (u, p, \psi)$

Replace $\tau$ in (2) with $\tau = \exp \psi$

$$\rho \left( \frac{\partial u}{\partial t} + u \cdot \nabla u \right) = \nabla p - 2 \eta_s \nabla \cdot D - \frac{\eta_p}{\Lambda} \nabla \cdot (\exp \psi),$$

$$\nabla \cdot u = 0,$$

$$\frac{\delta_a (\exp \psi)}{\delta t} + \frac{1}{\Lambda} (\exp \psi - 1) = 0,$$

Gradient of exponential of $\psi \rightarrow ???$

Solvers $\rightarrow ???$
LCR Formulation (I)

Experiences:

- Stresses grow exponentially
- Conformation stress is positive by design
- Stretching part creates numerical problem \( \left( \nabla u \sigma + \sigma \nabla u^T \right) \)

Idea ("Kupferman Trick"):

- Decompose the velocity gradient inside the stretching part
  \[ \nabla u = \Omega + B + N \sigma_c^{-1} \]

- Take the logarithm as a new variable \( \psi = \log \sigma \) using eigenvalue problem
  \[ \psi = R \log(\lambda) R^T \]
LCR Formulation (II)

Inside the constitutive equation (2), decompose

$$\nabla u = \Omega + B + N \sigma_c^{-1}
$$

$$\left( \frac{\partial}{\partial t} + u \cdot \nabla \right) \tau - (\Omega \tau - \tau \Omega) + 2B\tau = \frac{1}{\Lambda}(I - \tau)$$

(4)

Matrix $B$ is purely extension: Responsible for the stretching

$$\begin{bmatrix} b_1 & 0 \\ 0 & b_2 \end{bmatrix} \quad \text{... it is commutable !!!} \quad B\tau + \tau B = 2B\tau$$

Thus...

$$\frac{\partial \tau}{\partial t} = 2B\tau \quad \Rightarrow \quad \frac{\partial \psi}{\partial t} = 2B$$

Matrix $\Omega$ is purely rotation: Responsible for the rotating

$$\begin{bmatrix} 0 & -w \\ w & 0 \end{bmatrix} \quad \text{... it is symmetric !!!} \quad (\Omega \tau - \tau \Omega)_{ij} = (\Omega \tau - \tau \Omega)_{ji}$$

Thus...

$$\frac{\partial \tau}{\partial t} = (\Omega \tau - \tau \Omega) \quad \Rightarrow \quad \frac{\partial \psi}{\partial t} = (\Omega \psi - \psi \Omega)$$
LCR Formulation (III)

As in M. Behr, replace in (4) \( \tau = \exp(\psi) \) decouples 2Bτ

\[
\rho \left( \frac{\partial u}{\partial t} + u \cdot \nabla u \right) = \nabla p - 2 \eta_s \nabla \cdot \frac{\eta_p}{\Lambda} \nabla \cdot \exp(\psi),
\]

\[
\nabla \cdot u = 0,
\]

\[
\left( \frac{\partial}{\partial t} + u \cdot \nabla \right) \psi - (\Omega \psi - \psi \Omega) + 2B = \frac{1}{\Lambda} \left( e^{-\psi} - 1 \right),
\]

(5)

Note: Divergence of exponential of \( \psi \) is calculated explicitly using eigenvalue problem !!

Standard discretization techniques \( \Rightarrow \) EO, TVD
Standard nonlinear (Newton) and linear (MG) solvers
\( \Rightarrow \) Increases the critical Wi number dramatically !!
Numerical Results (steady problem tests)

1. Driven cavity

Velocity profile at the upper wall: \( v_{in} x^2(1-x)^2 \)

Dirichlet Bc’s everywhere

Stress field: Neuman Bc’s

\( v_{in} = 16 \)

2. 4 to 1 contraction

Velocity profile at the inlet:

\( \frac{3}{128} v_{in}(16 - y^2) \)

Out flow: Neuman Bc’s

Stress field: Neuman Bc’s

\( v_{in} = 1.0 \)
Lip-Vortex Growth

Cutline of $S_{11}$ at $y = 1$

Cutline if $\Psi_{11}$ at $y = 1$

-5.0 < $x$ < 5.0

-5.0 < $x$ < 5.0
Driven cavity

Velocity profile at the upper wall:

\[ v_{in} = x^2 (1 - x)^2 \]

\[ v_{in} = 8(1 + \tanh(8(t - 0.5))) \]

For \( t > 1 \), \( v_{in} = 16 \)

Dirichlet Bc‘s everywhere
Stress field: Neuman Bc‘s
Stream function

$\text{We} = 1$

$\text{We} = 3$

$t = 8$

Increasing $\text{Wi}$ number shifts the stream to the left
Increasing Wi number increases psi by a factor of 1
$\sigma_{11}$

$t = 8$

Re<<1  t=8 n=[64]

$W_{e} = 1$

$W_{e} = 3$
Increasing Wi number does not give much impact to the velocity field
Summary

With LCR, we are now able to simulate much higher Wi numbers

→ $\text{Wi} \sim 1.0$ for 4 to 1 configuration
→ $\text{Wi} \sim 0.5$ for square

NEW:

→ $\text{Wi} >> 4.5$ for 4 to 1 contraction (steady state)
→ $\text{Wi} >> 1.5$ for square (steady state)

Additional stabilization will help for high $\text{Re} + \text{Wi}$ numbers

→ LCR + Edge Oriented/TVD stabilization

Application to other viscoelastic flow models